Nuclear Data for Science and Technology (1988 MITO), 807- 810, Copyright © 1988 JAERI.

DEVELOPMENT OF NEUTRON DATA EVALUATION METHODS AND CREATING COMPLETE FILES OF ZIRCONIUM ISOTOPES

V. Bychkova, O. Grudzevich, A. Zelenetski, V. Plyaskin

IATE, Obninsk, USSR

Abstract: The evaluation of neutron cross-sections for Zirconium Isotopes is performed for the Soviet library of evaluated neutron data. The total, elastic, inelastic, radiative capture, (n,p), (n,α), (n,2n) and (n,n'p) reaction cross-sections and emission spectra are evaluated in the energy range from 10^{-5} ev to 20 MeV and given in the ENDF/B format. An evaluation in the resonance region is based on the experimental data. Theoretical model calculations are used for evaluation of excitation functions and particle emission spectra in a smooth cross sections region. Systematics of theoretical model parameters were used for decreasing the uncertainties of the evaluated data.

Introduction

The current trend in the development of neutron data evaluation methods has been towards taking into consideration as much experimental data as possible and using methods of consistent cross section calculations based on rigorous theoretical models. The present paper describes the use of such models and testing their parameters by experimental data to make complete files of evaluated neutron data for five stable isotopes of zirconium: ^{90}Zr, ^{91}Zr, ^{92}Zr, ^{94}Zr and ^{96}Zr. The evaluation made is in 10^{-5}eV through 20 MeV neutron energy range.

Experimental analysis

The first stage of any evaluation is analysing the experimental data collection for the nuclides in question. The data typically analysed are parameters of isolated neutron resonances, the discrete nuclear levels, neutron resonance density data, neutron elastic scattering cross sections as well as those for radiation capture, total neutron cross sections and threshold reaction cross sections, etc. It is at this stage that a comparative analysis of experimental data by different investigators and normalization of relatively measured values with regard to up to date nuclear standard values are made.

Neutron resonance parameters and discrete level data on individual nuclei are analysed to make sure that none of the resonances and levels has been overlooked or identified mistakenly. After that the values obtained are used both for deriving data on level density from Do(Bn) and No(Uo) and for evaluating neutron cross sections in the region of resolved resonances as well as evaluating inelastic neutron scattering cross sections and those of threshold reactions. The level density parameters a and S_{eff} were obtained using the generalized superfluid nuclear model /1/. Parameter a systematics was used as the first approximation for the nuclei with no experimental Do(Bn) available.

The first stage of evaluation was to get more exact optical potential parameters for neutrons, protons and alpha-particles using the spheroidal optical nuclear model. The neutron potential was tested by the SPRT method which consists in describing experimental data based on the neutron strength functions S_o and S_1. The potential scattering radius and σ_{tot} at low neutron energies.

So low neutron energy (E 200 keV) experimental data can be used to obtain both level density parameters and those of optical nuclear model. When the incident neutron energy is increased and the resonance structure becomes un resolved, the Hauser-Feshbach-Moldauer statistical nuclear reaction model is applied for experimental data analysis.

Use of statistical nuclear reactions model

The second stage of evaluation involves the analysis of experimental data by means of the statistical nuclear reac tions theory relations for those neutron energy regions where the unequilibrium processes contribution to the reaction cross section is negligible. The accuracy of level density parameters can be improved after extracting the value of $\rho_{exp}(U)$ from neutron emission spectra /2/. It is also possible to obtain more accurate neutron potential parameters based on the description of inelastic neutron scattering cross sections, as well as more accurate optical potential parameters for charged particles, based on the description of emission spectra in neutron-induced reactions. It is interesting to note that in many cases the above mentioned analysis indicates that in order to get a consistent description of the entire collection of experimental level density data available one should use the generalized superfluid nuclear model, rather than that of Fermi

gas /2,3/.

Unequilibrium processes in nuclear reactions

The nonstatistical component of nuclear reactions is often interpreted as the sum of direct transitions and multistage compound transitions /4/. The analysis of angular distribution of secondary particles shows that it is the direct mechanism that plays the leading part in forming nonstatistical component of reaction cross sections. To describe various experimental data a much simpler exciton preequilibrium particle emission model is widely used /5/ alongside with the rigorous theoretical approaches. The paper /6/ however shows that the exciton model fails to give a consistent description of nucleon emission spectra in inelastic scattering and charge exchange reactions because of the inelastic scattering being affected by the direct excitation of collective levels in the target nucleus.

At the third stage of evaluation the direct, preequilibrium and statistical nuclear reaction mechanisms are consistently taken into account to describe the entire experimental data collection for the group of nuclei in question with unified set of model parameters. The direct processes contribution to the discrete collective levels excitation functions is taken into consideration according the generalized optical nuclear model with experimental parameters β_λ of dynamic deformation as well as adequately chosen phenomenological neutron optical potential parameters. The weak interaction method with accurate choice of the core is used for odd-A nuclei. In case there are no experimental β_λ available the systematics of the direct processes integral contribution into inelastic neutron scattering from /6/ is used.

So it is at the first three stages that consistent description is obtained of the entire experimental data collection for the nuclides under consideration. To get more unified model parameters the same set of parameters is used for describing experimental cross sections for neighbouring nuclei which confirms the method's predictive capabilities.

Creating complete files of Zr isotopes

The following section describes briefly the information contained in the complete files of the five stable zirconium isotopes. The complete files we created are part of the Soviet library /8/.

Evaluated neutron data libraries known at present use the ENDF/B format which includes two fundamentally different neutron energy regions, i.e. the region of resonance cross sections and the region of smooth ones. The division reflects the nature of neutron cross sections energy dependence and on the other hand the way evaluated neutron data are presented in the format. The actual cross sections are set up to some energy scale in the smooth cross sections region while resonance parameters from which the cross sections will be recovered are set up in the resonance region.

The resonance energy region differs radically from the smooth cross section region as far as evaluation is concerned Resonance cross sections evaluating is based upon extracting neutron resonance widths from experimental data on transmission and extracting radiation widths from radiation capture cross section measurements, neutron widths given. The position of individual resonances as well as their other characteristics are derived from the entire experimental data collection. No evaluation of the detailed course of the cross sections in the resonance region can be obtained without experimental information about the parameters of individual resonances.

Basically advances in evaluating resonance cross sections are, therefore, determined by expanding experimental data in this energy region and getting more accurate data.

The up-to-date experimental data /9/ on the neutron resonance parameters of zirconium isotopes have been obtained from both transmission and radiation capture measurement experiments. The resolved resonance region upper limit which is determined by the experiment's energy resolution and the properties of the nuclei involved has increased considerably. In determining this limit it is essential not to include in the resonance region the bands where some of the resonances are missing from the experimental data. It is generally believed that a considerable number of resonances having been left out is indicated by a bend in cumulative level number.

Included in the table below are the energies of the resolved resonances upper region (line 1), the parameters of the resonances being included in the complete files of evaluated data for the five stable zirconium isotopes. The values of radiation, neutron, and total widths, energies for S and p-resonances are taken from the compilation /10/. Average values were assigned to the individual resonances where radiation widths were not available.

The Breit-Wigner multilevel formalism was used to reconstruct the detailed course of the resonance cross-sections curve. The correctness of cross-sections evaluation in the resonance region is checked by calculating the cross-sections at the thermal point and the resonance capture integral as well as the average cross sections (n,γ) comparing with poor resolution experimental data. The comparison of calculated values for $\sigma_{n\gamma}^{o}$ and I_γ from the table with the experimental ones proves the Breit-Wigner formalism being able to reproduce the detailed course of the cross sections well.

As the incident neutron energy in-

Table. Resonance Energy Region Characteristics of Complete Neutron Data Files for Zirconium Isotopes.

		^{90}Zr	^{91}Zr	^{92}Zr	^{94}Zr	^{96}Zr
1	E_{res}, keV	200	30	85	90	30
2	N_{res}	88	140	86	73	
3	$S_{\gamma\ calc}$, 10^{-4}	0,1	2,15	0,38	0,3	
4	$S_{\gamma\ exp}$, 10^{-4}	0,4	2,0	0,5	0,4	
5	$S_{\gamma\ calc}$, 10^{-4}	0,7	1,0	1,83	1,1	
6	$S_{\gamma\ exp}$, 10^{-4}	1,3	7,0	1,9	1,0	
7	$D_{o\ exp}$, keV	6,4±1,1	0,57±0,1	2,6±0,7	3,6±0,8	13±4
8	$\langle\Gamma_\gamma\rangle_{o\ exp}$, meV	240	140	140	130	
9	$\langle\Gamma_\gamma\rangle_{o\ exp}$, meV	440	240	360	185	
10	E_{unres}, keV	400	200	200	200	
11	$\sigma^{o}_{n\gamma\ exp}$, mb	11±6	1240±250	220±60	49,9±2,4	22,9±1
12	$\sigma^{o}_{n\gamma\ calc}$, mb	10	1200	200	50	20
13	$I_{\gamma\ exp}$, mb		5200±700		230±10	5300±300
14	$I_{\gamma\ calc}$, mb	140	5000	630	235	5200
15	$S_{o\ exp}$	0,7±0,2	0,36±0,08	0,5±10	0,5±0,15	0,34±0,14
16	$S_{1\ exp}$	4,0±0,6	6,7±1,3	7,0±1,3	9,6±2,0	6,0±1,8

creases it becomes imposible to resolve the individual resonances in the experiment. In this case the observed cross sections corresponding to the so-called unresolved resonances region are quite smooth, nevertheless they still contain information on the resonance structure.

The ENDF/B-5 format used for creating the files allows the unresolved resonances region to be entered, the average resonance parameters being entered depending on the energy. It is essential that on the one hand the parameters should correspond to the average resonance parameters and on the other hand reconstruct the observed cross sections. It is necessary to present the average interval between the resonances and the average radiotion and neutron widths as a function of the energy.

The choice of the unresolved resonances upper boundary is a compromise between the desire to put it as high as possible to get a better picture of cross sections resonance self-shielding factor and the necessity to limit oneself to neutron energies where the contribution of the neutrons with the orbital angular momentum l=3 to cross sections is yet insignificant. The problem is that the ENDF/B-5 format does not permit the f-wave to be set explicitly and its contribution to the cross section is usually compensated by the introduction into the cross section smooth back-ground which naturally should not be too large as compared with the magnitude of the observed cross section.

The unresolved resonances region that have been adopted for the newly-created files of evaluated neutron data on the zirconium isotopes are shown in table.

So the analysis we have just described helped create section 2151 of the complete files of evaluated neutron data on the five stable zirconium isotopes, which corresponds in the ENDF/B-5 format to the resonance cross sections region composed of the resolved resonances region and the unresolved resonances region. Fixed values in the resolved resonances region are the parameters of individual resonances, namely, the energy, the total angular momentum and parity, the orbital angular momentum, the radiation, neutron and total widths. To reconstruct the detailed course of the cross sections the Breit-Wigner multilevel formalism was used. The unresolved resonances region is represented by average resonance parameters and the cross sections can be reproduced by means of the Hauser-Feshbach-Moldauer relations.

As the neutron energy increases the width of the resonances increases and the distance between the resonances decreases. As a result the resonances begin to overlap and the experiment produce cross sections determined by the contribution of many resonances. The methods of calculating cross sections in this energy region are known quite well.

They are based upon the use of the generalized optical, preequilibrium, statistical models describing the contribution to the reaction cross section by the direct, preequilibrium and statistical reaction mechanisms.

The possible interference of the direct and statistical reaction mechanisms contribution may cause certain difficulties in combining correctly the generalized optical model, by which collective levels excitation cross sections are calculated, with the statistical model /6/. However, when the number of the channels is increased and the parameters of the quadrupole dynamic deformation of the collective levels are small, the direct and the statistical parts of the cross section can be added incoherently /11/. This is the case for all zirconium isotopes. The first step in calculating the cross sections was determining the S-matrix by means of the coupled-channel method in order to obtain the part of the cross sections due to direct interaction. This was followed by calculations based on the preequilibrium and statistical models with a corresponding decrease in the absorption cross section by the value of the direct reaction mechanism cross section. So spheroidal optical nuclear model can be used in calculations based on the Hauser-Feshbach relations, and the direct reaction mechanism's contribution can be calculated by means of the coupled-channel method within the framework of the generalized optical model.

The evaluation technique we have just described was used to create evaluated nuclear data files for the stable zirconium isotopes. The files will be presented to the Nuclear Data Centre (Obninsk) in 1988.

REFERENCES

1. O.T. Grudzevich et al: International Conference on Neutron Physics, Kiev, (1987)
2. O.T. Grudzevich et al: In Proc. 2nd Meet. of the IAEA Coord. Research., IAEA Vienna (1988)
3. V.M. Bychkov et al: ibid /2/
4. H. Feshbach: Ann. Phys. 125, 429 (1980)
5. T.J. Griffin: Phys. Rev. Lett. 17, 478(1966)
6. O.T. Grudzevich et al: In Proc. of the IAEA. Research Coordination Meeting on Methods for the calculations of neutron nuclear data for structural materials, Bologna, (1986) IAEA, 81(1988)
7. O.T. Grudzevich et al: In Proc. 2nd of IAEA Coord. Research Prog., IAEA Vienna (1988)
8. V.V. Bychkova et al: International Conference on Neutron Physics, Kiev (1988)
9. S.F. Mughabghab et al: Neutron Cross Sections v.1 part A, N.Y. - London, Academic Press (1981)
10. T.S. Belanova et al: Radiactive Capture of Neutrons (Russian) M., Energoatomizdat (1986)
11. V.M. Bychkov et al: Proc. of the 4-th All-Union Conf. on Neut. Phys., Kiev, 2, 84(1977)